Heisenberg model in a random field: phase diagram and tricritical behavior

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Abstract

By using the differential operator technique and the effective field theory scheme we study the tricritical behavior of Heisenberg classical model of spin-1/2 in a random field. The phase diagram in the T-h plane on a square and simple cubic lattice for a cluster with two spins is obtained when the random field is bimodal distributed.

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1. Introduction

The random field Ising model (RFIM) has been investigated extensively both theoretically and experimentally in last years.[1 −4] Some questions such as the lower critical dimension and the existence of a static phase transition have been already solved from the theoretical point of view, but others questions as the existence of the tricritical point are still open. However, it is now understood that RFIM describes the essential physics of a rich class of experimentally accessible disordered systems. These include structural phase transitions in random alloys, commensurate charge-density-wave systems with impurity pinning, binary fluid mixtures in random porous media, and the melting of intercalates im layered compounds such as TiS_2. The behavior of the RFIM is governed by the competing tendencies of the spins to align ferromagnetically under impetus of the exchange or to follow local fields and so be uncorrelated.

The RFIM has been studied with different methods. The renormalization-group theory (RG) of phase transition and critical phenomena represent one of most powerful tool of theoretical physics in last decades. Until then (early 1970s) all calculations of critical exponents were made either by exactly or by series expansions. Therefore, employing the renormalization-group arguments (which can be applied for weak fields), the proof of the equivalence between an Ising ferromagnet in a random field and a dilute antiferromagnet in a uniform field has been demonstrated. These question have been very explored (see 5 and references therein).

In the RG scheme, such as, the effective field RG (EFRG)[6,7] and the Mean-field RG (MFRG)[8,9] methods have been successfully employed in spin systems, where the results obtained are in accordance with other more effective approach (series expansion, Monte Carlo simulation among others). Those approaches (MFRG and EFRG) are based on comparison of two clusters of different sizes, each of them simulating infinite systems. On the other hand, the mean field approximation (MFA) has been extensively applied in the study of RFIM. The MFA provides very interesting results about RFIM. For example, a bimodal

distribution for random field gives rise to a tricritical point and consequently first order phase transitions, at very low temperatures for certain values of field strength, but does not occur in the case of a gaussian distribution.[10−14] In addition, it is possible to establish a complete mapping between the parameters of the Ising ferromagnet in a random field and the dilute Ising antiferromagnet in a uniform field.

By employing the same strategy of EFRG, the effective field theory (EFT) has been used to study cooperative phenomena and phase transitions in various systems and giving useful qualitative and quantitative insights for the critical behavior of a wide variety of classical and quantum lattice spin systems.[15−17] The approach of EFT uses, as a starting point, the rigorous Callen-Suzuki spin identities (See Refs. 18 and 19) and the effects of the surrounding spins on each cluster are taken into account by using a convenient differential operator technique introduced by Honmura and Kaneyoshi.[20] In this procedure, all relevant self-spin correlations are taken exactly into account in the EFT equation of state.[21] Therefore, the EFT approach is superior to the standard MFA.

In this work, we study the behavior of phase diagram (in $T - h$ plane) for Heisenberg classical model of spin-1/2 on a square and simple cubic lattice by employing a bimodal probability distribution for random fields in a cluster with two spins by using the result recently obtained on diluted systems.[6] The outline of the remainder of this paper is as following: in section **1**, the formalism and calculations are developed and the results and conclusions are presented in section **2**.

2. Formalism and Calculations

The system to be studied is the n-vectorial model in a random field described by the Hamiltonian

$$- \beta \mathcal{H} = K \sum_{(i,j)} \mathbf{S_i} \cdot \mathbf{S_j} + \sum_i \mathbf{h_i} \cdot \mathbf{S_i}, \tag{1}$$

where the summation is performed over all pairs of the nearest-neighboring sites (i, j). The quantities $\mathbf{S_i}$ are isotropically interacting n -dimensional classical spins of magnitude $\sqrt{n}$ localized on site i and the Cartesian components of $\mathbf{S_i}$ obeys the normalization condition,[23]

$$\sum_{u}^{n}(S_i^n)^2 = n.$$

K [$\equiv J/k_B T$, k_B is the Boltzmann constant and T the temperature] is the exchange interaction between the spins, h_i [$h \equiv \mu_B H/k_B T$, where μ is the Bohr magneton and H is the random magnetic field] is the reduced random magnetic field at site i with probability distribution

$$P(h_i) = \frac{1}{2}[\delta(h_i + h) + \delta(h_i - h)]. \tag{2}$$

Hamiltonian (1) reduces to the $S = \frac{1}{2}$ Ising, planar (XY), Heisenberg and spherical models for $n = 1, 2, 3$ and ∞, respectively.

In this work, we follow the EFT procedure (see Ref. 16) to study the critical properties of the Hamiltonian described by Eq.(1) by employing the axial approximation.[22] Since the Hamiltonian for a cluster with two spins can be written as

$$H = K\mathbf{S}_1 \cdot \mathbf{S}_2 + a_1 \cdot S_1^1 + a_2 \cdot S_2^1, \tag{3}$$

where $a_l = h_l + K\Sigma_{j\neq l}^{z-1}S_j^1$, $(l = 1, 2)$ and z is the lattice coordination number.

The average magnetization per-spin $m = \frac{1}{2}\langle(S_1^1 + S_2^1)\rangle$ for cluster with two spins is given by (See Refs. 6 and 9)

$$m = \langle \prod_{k\neq 1,2}^{z-1} (\alpha_x + S_k^1\beta_x) \prod_{l\neq 1,2}^{z-1} (\alpha_y + S_l^1\beta_y)\rangle g_n(X,Y)|_{X=h_1,Y=h_2}. \tag{4}$$

$\alpha_\nu = \cosh(KD_\nu)$, $\beta_\nu = \sinh(KD_\nu)$, $(\nu = x, y)$, $X(Y) = x(y) + h_1(h_2)$. D_ν $(\equiv \frac{\partial}{\partial\nu})$ is differential operator which satisfy the mathematical relation

$$sinh(aD_x + bD_y)g_n(X,Y)|_{X=h_1,Y=h_2} = g_n(a + h_1, b + h_2),$$

where $g_n(X,Y)$ is given by

$$g_n(X,Y) = \frac{\sinh(X+Y)}{\cosh(X+Y) + \exp(-2K)M_n(K)\cosh(X-Y)}, \tag{5}$$

and

$$M_n(K) = \frac{I_{n/2}(nK) - I_{n/2-1}(nK)}{I_{n/2}(nK) + I_{n/2-1}(nK)}.$$

Here $I_n(X)$ is a modified Bessel function of the first kind. Eq. (4) is exact and will be applied here as a basis of our formalism, since it yields the cluster magnetization m and the corresponding multi-spin correlation functions associated with various sites for the cluster under consideration. Here we apply the EFT approximation in both sides of Eq. (4), i.e., the thermal and random average (denoted by $\langle \cdots \rangle_c$), along with the decoupling procedure which ignores all high-order spin correlations, namely $\langle S_i^1 S_j^1 \cdots S_n^1 \rangle_c \approx \langle S_i^1 \rangle_c \langle S_j^1 \rangle_c \cdots \langle S_n^1 \rangle_c$, with $i \neq j \neq \cdots \neq n$. Based on this approximation and replacing each boundary configurational spin average by the symmetry breaking mean-field parameters b_i for all i, one set up the equation of state for $\bar{m} = \langle m \rangle_c$. By using the properties of differential operator and assuming translational invariance, we obtain for the square (sq) and simple cubic lattice (sc), respectivelly,

$$\bar{m} = \sum_{k=1}^{6} A_{k,sq}(K,n,h)\bar{m}^k, \tag{6}$$

$$\bar{m} = \sum_{k=1}^{10} A_{k,sc}(K,n,h)\bar{m}^k. \tag{7}$$

The coefficients $A_{k,(sq,sc)}(K,n,h)$ [$k = $ even] are zero to satisfy the time reversal symmetry of the Ising model, as well the properties of differential operator technique.

3. Results and Conclusions

In this section we apply the conditions for determining of the second-order transition line and the tricritical point (TCP) in the $n-$ vector model in a random field. We will focus on the case $n = 3$, which corresponds to the Heisenberg classical model of spin-1/2.

In the vicinity of the second-order phase transition, the Eqs. (6 - 7) is given by

$$\bar{m}^2 = -\frac{A_{1,(sq,sc)}(K,n,h) - 1}{A_{3,(sq,sc)}(K,n,h)}. \tag{8}$$

Since the magnetization ($\bar{m}$) goes to zero continuously, to obtain the second order phase transition line, in the $T - h$ plane, we need solve the equations

$$A_{1,(sq,sc)}(K,n,h) = 1, \qquad A_{3,(sq,sc)}(K,n,h) < 0. \tag{9}$$

On the other hand, the r.h.s. of Eq. (8) must be positive; otherwise, the transition is interpreted to be of first-order. Unfortunately the first order transition line cannot to be analyzed in the frame of the differential operator technique, therefore we have confined our calculations only to the second order transitions, including the TCP. We obtain the TCP by solving the equations

$$A_{1,(sq,sc)}(K,n,h) = 1, \qquad A_{3,(sq,sc)}(K,n,h) = 0. \tag{10}$$

The numerical solution of Eq. (9) provide the second-order phase transition line which is shown in Figure 1. When the random field is zero, we obtain the well-known critical temperature of Heisenberg classical model of spin-1/2, $K_{c,sq}^{-1} = 3.005$ and $K_{c,sc}^{-1} = 5.031$. In Figure 1, the solid line indicate the second-order phase transitions; the black diamonds denote the position of the TCP at which phase transition changes from second to first order. The numerical solution of Equations (10) provide the values for the tricritical points $(h_{TCP}, K_{TCP}^{-1}) = (1.800, 0.958)$ and $(h_{TCP}, K_{TCP}^{-1}) = (2.785, 2.389)$ for the square and simple cubic lattice, respectivelly. We might conclude saying that EFT approximation is able to predict the presence of tricritical behavior for the Heisenberg classical model of spin-1/2 on a square and simple cubic lattice in a random magnetic field which takes on the random values

$\pm h$ with equal probabilities. As can be seen, our results show the existence of the TCP for square lattice ($z = 4$) in accordance with mean-field[24] and Betthe-Peierls[25] approximations. This occur because to obtain the first-order phase transition we must have at least the $\bar{m}^5$ term in the expansion of Eqs.(6 - 7). Therefore, in the presente approach we cannot observe behavior tricritical for lattice with coordination numbers $z < 4$.

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Figure Captions:

Figure 1. Phase diagram for Heisenberg classical model in presence of the random magnetic field, in the $T - h$ plane, on a square (sq) and simple cubic (sc) lattice.